Charge stripe order from antiphase spin spirals in the spin-Fermion model

Marcello B. Silva Neto[1]

[1] *Institut für Theoretische Physik III, Universität Stuttgart, Pfaffenwaldring 57, 70550, Stuttgart, Germany.*

We revisit the ground state of the spin-Fermion model within a semiclassical approximation. We demonstrate that antiphase spin spirals, or π-spirals, whose chirality alternates between consecutive rows (or columns) of local moments, have, for sufficiently high carrier concentration, lower energy than the traditional Shraiman and Siggia spirals. Furthermore, π-spirals give rise to modulated hopping, anisotropic 1D transport, and charge density wave formation. Finally, we discuss the relevance of π-spirals to the physics of charge stripe formation in cuprates, such as $La_{2-x}Sr_xCuO_4$.

PACS numbers: 74.25.Ha, 75.10.Jm, 74.72.Dn

I. INTRODUCTION

The determination of the ground state of a strongly correlated system where conduction electrons interact with local magnetic moments is an issue that is relevant to many different areas of condensed matter physics. The usual starting point for such study is the so called Kondo lattice model (KLM), where the local moments are assumed to form a regular lattice. The KLM has become the paradigm for the study of the physics of heavy Fermion (HF) compounds and has been extensively investigated both theoretically and with numerical methods (for recent references see, for example, Refs. 1 and 2). When generalized to include a Heisenberg superexchange interaction, J, that favours antiferromagnetic ordering among nearest neighbour local moments, the generalized KML, or yet, the spin-Fermion (SF) model, has been argued to capture the essential physics of the high temperature superconductors (HTSC).[3]

Within the framework of the HTSC, the conduction electrons in the SF model are provided by the holes doped into the p_x and p_y orbitals of the O^{--} ions, while the local moments are provided by the incomplete $3d_{x^2-y^2}$ shell of the Cu^{++} ions. Although this microscopic picture is by now well established, after 20 years of intense theoretical and numerical research[4] the ground state of the HTSC is not yet completely understood. It is believed that the true nature of the ground state is determined by the competition between the different energy scales of the model: the hopping integral, t, the Kondo coupling, J_K, and the antiferromagnetic superexchange, J, as well as by disorder. A large number of possible ground states have been obtained in the literature, including phase separation,[5] charge stripes formation,[6] and spiral magnetic order,[7,8] among others.

From the experimental point of view, inelastic neutron scattering experiments within the superconducting phase of $La_{2-x}Sr_xCuO_4$, $x > 5.5\%$, revealed that dynamical incommensurate (IC) spin correlations coexist with superconductivity[9]. In addition, it has also been observed experimentally the existence of IC "charge" peaks accompanying the IC magnetic order, with twice the incommensurability of the magnetic one.[10] These results were immediately and consistently interpreted as evidence of the formation of charge stripes that act as antiphase domain walls,[6] and apparently rule out other possible ground states such as Shraiman-Siggia spirals,[7] which, despite being able to explain the IC magnetic order, require a uniformly charged ground state.[11]

In this brief report we revisit the ground state of the SF model for cuprate superconductors within a semiclassical approximation. We demonstrate that antiphase spin spirals, or π-spirals, whose chirality alternates between consecutive rows (or columns) of local moments, have, for sufficiently high carrier concentration, lower energy than the traditional Shraiman and Siggia spirals. Furthermore, π-spirals give rise not only to IC magnetism but also to modulated hopping, anisotropic 1D transport, and charge density wave (CDW) formation. Thus, our theoretical results indicate, for the first time, the possibility of the *coexistence* between spiral magnetic order and CDW formation, in agreement with recent quantum Monte Carlo simulations for the SF model.[12] Finally, we discuss the relevance of π-spirals to the physics of charge stripe formation in the low temperature tetragonal phase of cuprate superconductors, such as $La_{2-x}Sr_xCuO_4$.

II. THE SPIN-FERMION MODEL

The Hamiltonian for the spin-fermion model can be written as $H = H_t + H_K + H_J$ where

$$
\begin{aligned}
H_t &= -t \sum_{\langle i,j\rangle,\alpha} (p^\dagger_{i,\alpha} p_{j,\alpha} + h.c.) - \mu \sum_{i\alpha} p^\dagger_{i,\alpha} p_{i,\alpha} \\
H_K &= \frac{J_K}{2} \sum_{i,\alpha,\beta} \mathbf{S}_i \cdot p^\dagger_{i,\alpha}\, \sigma_{\alpha\beta}\, p_{i,\beta} \\
H_J &= J \sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \qquad (1)
\end{aligned}
$$

$p^\dagger_{i,\alpha}$ creates a hole at the site i with spin projection α, t is the nearest-neighbour hopping integral, J_K is an antiferromagnetic exchange interaction between the Cu^{++} local moment and the spin of the doped O^{--} holes, J is the Heisenberg antiferromagnetic superexchange, and μ is the chemical potential. In the large J_K/t limit, the above Hamiltonian is known to reduce to the $t-J$ model.

Since conduction electrons and local moments in the SF model are independent degrees of freedom we can treat the local moments classically without affecting the mobile Fermions.[13] This is the basis of the semiclassical approximation used here. In this case, the Hamiltonian becomes quadratic in the Fermion fields and can be diagonalized. For simplicity we choose a spin-quantization basis such that $\mathbf{S}_i = (0, 0, S)$ at every site, and the Kondo term reduces to a shift on the chemical potential for the different spin components of the doped holes, $H_K = (J_K/2)S\sum_i (p^\dagger_{i,\uparrow} p_{i,\uparrow} - p^\dagger_{i,\downarrow} p_{i,\downarrow})$.

As it was originally proposed long ago by Shraiman and Siggia,[7] for $t > J$ (for $La_{2-x}Sr_xCuO_4$ $t/J \approx 3$) the hopping of the doped holes is favoured by a noncollinear configuration for the local moments of the spiral type (see also Ref. 14). Because of our choice for the local spin-quantization basis, as the spins spiral so does the local frame. This will affect the mobile holes that transform under the following SU(2) transformation

$$U(\mathbf{x}_i) = e^{\mathrm{i}\theta_i \zeta\cdot\vec{\sigma}/2} = \cos\frac{\theta_i}{2} + \mathrm{i}\,\vec{\sigma}\cdot\zeta \sin\frac{\theta_i}{2}. \qquad (2)$$

Here ζ is a unitary vector pointing to an arbitrary direction in the plane perpendicular to the local spin, and $\vec{\sigma}$ are the Pauli matrices. Under such SU(2) transformation the Fermion fields are then transformed as

$$\begin{pmatrix} p_{i,\uparrow} \\ p_{i,\downarrow} \end{pmatrix} = U^\dagger(\mathbf{x}_i) \begin{pmatrix} c_{i,\uparrow} \\ c_{i,\downarrow} \end{pmatrix}, \qquad (3)$$

and we usually write

$$\theta_i = \mathbf{q}\cdot\mathbf{x}_i, \qquad (4)$$

in such a way that the classical AF Néel state is parametrized by $\mathbf{q} = (\pi, \pi)$ and has classical energy $E_{AF} = -4NJS^2$, where N is the total number of local moments.

III. INPHASE OR 0-SPIRALS

Inphase or 0-spirals are parametrized as having an IC wave vector given by, for example,

$$\mathbf{q} = (q_x, \pi). \qquad (5)$$

This corresponds to Shraiman-Siggia original solution[7] (see Fig. 1) and in this case the SF model reduces to

$$\begin{aligned} H_t &= -t\sum_{\langle i,j\rangle,\alpha} \cos\left(\frac{\mathbf{q}\cdot(\mathbf{x}_i - \mathbf{x}_j)}{2}\right)(c^\dagger_{i,\alpha} c_{j,\alpha} + h.c.) \\ &\quad - t\sum_{\langle i,j\rangle} \sin\left(\frac{\mathbf{q}\cdot(\mathbf{x}_i - \mathbf{x}_j)}{2}\right)(\mathrm{i}e^{-\mathrm{i}\zeta} c^\dagger_{i,\uparrow} c_{j,\downarrow} - \mathrm{i}e^{\mathrm{i}\zeta} c^\dagger_{j,\uparrow} c_{i,\downarrow}), \\ H_K &= \frac{J_K S}{2}\sum_i (c^\dagger_{i,\uparrow} c_{i,\uparrow} - c^\dagger_{i,\downarrow} c_{i,\downarrow}), \\ H_J &= -2NJS^2\left[1 - \cos q_x\right]. \end{aligned} \qquad (6)$$

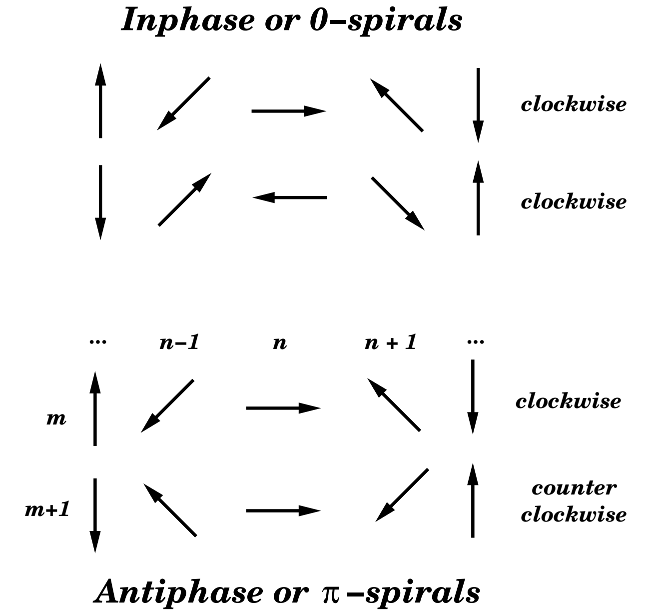

FIG. 1: Inphase (top) and antiphase (bottom) spiral configurations for the magnetic ground state of the spin-Fermion model. For inphase $(1, 0)$ spirals all spins rotate clockwise, for example, in every row m of copper ions. For antiphase $(1, 0)$ spirals, on contrary, the sense of rotation alternates between two consecutive rows, m and $m + 1$ for example.

The spiraling of the local moments favours the hopping of the conduction electrons in the direction of the pitch of the spiral via the H_t term, at the price of some magnetic energy loss (H_J in Eq. (6) is larger than $-4NJS^2$). In momentum space the above Hamiltonian reads

$$H = \sum_{\mathbf{k}} (\, c^\dagger_{\mathbf{k},\uparrow} \;\; c^\dagger_{\mathbf{k},\downarrow}\,) \begin{pmatrix} \xi_0(\mathbf{k}) + \frac{J_K S}{2} & \xi_2(\mathbf{k}) \\ \xi_2(\mathbf{k}) & \xi_0(\mathbf{k}) - \frac{J_K S}{2} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k},\uparrow} \\ c_{\mathbf{k},\downarrow} \end{pmatrix}, \qquad (7)$$

where

$$\begin{aligned} \xi_0(\mathbf{k}) &= -2t\cos k_x \cos\frac{q_x}{2}, \\ \xi_2(\mathbf{k}) &= -2t\left[\sin k_x \sin\frac{q_x}{2} + \sin k_y\right]. \end{aligned} \qquad (8)$$

The above Hamiltonian can be diagonalized in momentum space and we obtain the dispersions

$$\epsilon^\pm_0(\mathbf{k}) = \xi_0(\mathbf{k}) \pm \sqrt{\xi_2^2(\mathbf{k}) + \left(\frac{J_K S}{2}\right)^2}, \qquad (9)$$

with energy minima are located near $\mathbf{k}_0 = (\pi/2, \pi/2)$ and symmetry related points in the magnetic Brillouin zone.

We now calculate the total energy of the 0-spiral ground state. It is clear that, although the system pays magnetic energy in order to stabilize the 0-spiral, the gain in kinetic energy

$$E^0_{kin} = \sum_{\mathbf{k}} \epsilon^-_0(\mathbf{k})\Theta(\mu - \epsilon^-_0(\mathbf{k})), \qquad (10)$$

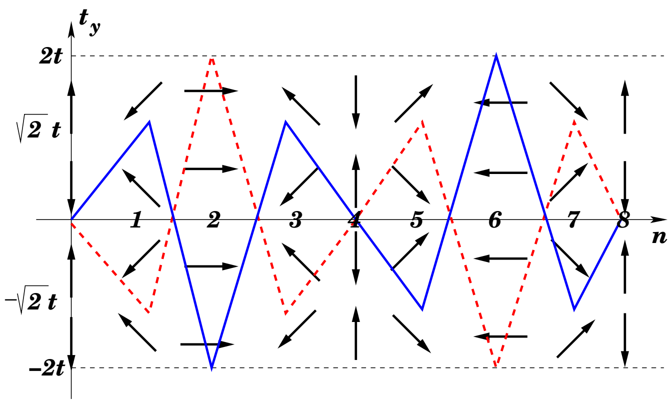

FIG. 2: (Color online) Modulated hopping amplitudes for the two degenerate antiphase or π-spiral configurations at filling $\delta = 1/8$. The blue (solid) curve is the hopping amplitude when the spins in the top row rotate clockwise (case drawn) while the red (dashed) curve is the hopping amplitude when the spins in the top row rotate counter-clockwise (not shown).

is *always larger* than the magnetic energy loss, already for infinitesimal doping (as it has been demonstrated in Ref. 15, a Dzyaloshinskii-Moriya term, not considered here, can shift this instability to finite doping, thus stabilizing the Néel ground state). Here we assumed that only the lower energy band in Eq. (9) is filled, due to the large gap $(J_K S)/2$ (recall that $J_K/t \gg 1$), and we used that $k_F = \sqrt{2\pi\delta}$, where δ gives the carrier concentration.

The are two problems with the 0-spiral state: i) it does not break translational invariance in the charge sector, as it is observed experimentally;[10] ii) it favours the transport in the direction *parallel* to the pitch of the spiral, while experiments have demonstrated that the anisotropic 1D transport should be *perpendicular* to it.[16] As we shall demonstrate now, both issues are naturally incorporated by the antiphase or π-spiral state.

IV. ANTIPHASE OR π-SPIRALS

Antiphase or π-spirals can be parametrized by the IC wave vector

$$\mathbf{q}_m = ((-)^m q_x, \pi), \tag{11}$$

where m labels a certain row of Cu^{++} ions, see Fig. 1. The spin-Fermion model in this case is rewritten as (m and n label, respectively, rows and columns of local moments)

$$\begin{aligned}
H_t &= -t \sum_{m,n,\alpha} \cos\frac{q_x}{2} (c^\dagger_{(m,n+1)\alpha} c_{(m,n)\alpha} + h.c.) \\
&- \; t \sum_{m,n,\alpha} \sin(nq_x) (c^\dagger_{(m+1,n)\alpha} c_{(m,n)\alpha} + h.c.) \\
&+ \; t \sum_{m,n} \cos(nq_x) (\mathrm{i}e^{-\mathrm{i}\zeta} c^\dagger_{(m+1,n)\uparrow} c_{(m,n)\downarrow} + h.c.) \\
&+ \; t \sum_{m,n} \cos(nq_x) (\mathrm{i}e^{\mathrm{i}\zeta} c^\dagger_{(m+1,n)\downarrow} c_{(m,n)\uparrow} + h.c.) \\
H_K &= \frac{J_K S}{2} \sum_{m,n} (c^\dagger_{(m,n)\uparrow} c_{(m,n)\uparrow} - c^\dagger_{(m,n)\downarrow} c_{(m,n)\downarrow}) \\
H_J &= 2NJS^2 \cos q_x .
\end{aligned} \tag{12}$$

There are important differences with respect to the case of the 0-spirals: i) in the π-spiral ground state, the spin independent part of the hopping *perpendicular* to the spiral pitch becomes *modulated*, see Fig. 2; ii) it becomes maximal for parallel configurations of the local moments, as in positions $n = 2, 6$; iii) it vanishes for antiparallel configurations for the local moments, as in positions $n = 0, 4, 8$. Furthermore, the modulation in the vertical hopping leads to a modulation on the carrier density, and, as a consequence, to a CDW instability of the stripe sort.[6] Finally, it is clear that the vertical hopping can be much larger than the horizontal one, thus exposing the 1D nature of the transport in the π-spiral phase.

We still have to show that the π-spiral phase has lower energy than the 0-spiral one. In momentum space the Hamiltonian reads

$$H = \sum_{\mathbf{k}} (\, c^\dagger_{\mathbf{k},\uparrow} \;\; c^\dagger_{\mathbf{k}+\mathbf{q},\uparrow} \;\; c^\dagger_{\mathbf{k},\downarrow} \;\; c^\dagger_{\mathbf{k}+\mathbf{q},\downarrow} \,) \begin{pmatrix} \xi_0(\mathbf{k}) + \frac{J_K S}{2} & -\Delta(\mathbf{k}) & e^{-\mathrm{i}\zeta}\xi_2(\mathbf{k}) & e^{-\mathrm{i}\zeta}\Delta(\mathbf{k}) \\ -\Delta(\mathbf{k}) & \xi_0(\mathbf{k}+\mathbf{q}) + \frac{J_K S}{2} & e^{-\mathrm{i}\zeta}\Delta(\mathbf{k}) & e^{-\mathrm{i}\zeta}\xi_2(\mathbf{k}+\mathbf{q}) \\ e^{\mathrm{i}\zeta}\xi_2(\mathbf{k}) & e^{\mathrm{i}\zeta}\Delta(\mathbf{k}) & \xi_0(\mathbf{k}) - \frac{J_K S}{2} & -\Delta(\mathbf{k}) \\ e^{\mathrm{i}\zeta}\Delta(\mathbf{k}) & e^{\mathrm{i}\zeta}\xi_2(\mathbf{k}+\mathbf{q}) & -\Delta(\mathbf{k}) & \xi_0(\mathbf{k}+\mathbf{q}) - \frac{J_K S}{2} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k},\uparrow} \\ c_{\mathbf{k}+\mathbf{q},\uparrow} \\ c_{\mathbf{k},\downarrow} \\ c_{\mathbf{k}+\mathbf{q},\downarrow} \end{pmatrix}. \tag{13}$$

The above Hamiltonian can be diagonalized and the new dispersions are

$$\epsilon_\pi^{(\pm,\pm)}(\mathbf{k}) = \pm\sqrt{F_I(\mathbf{k}) \pm 2\sqrt{F_{II}(\mathbf{k})}}, \tag{14}$$

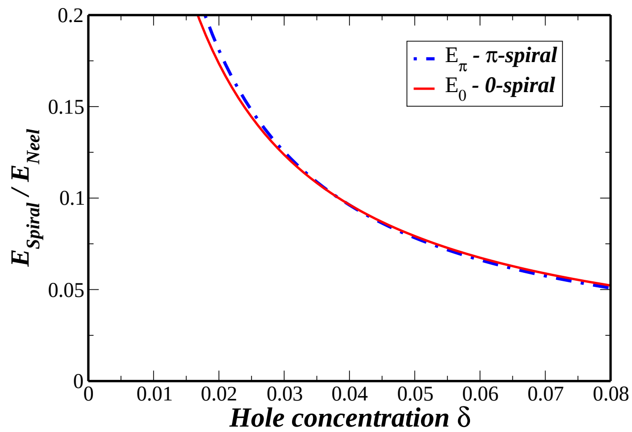

FIG. 3: Doping dependence of the energy of both inphase or 0-spirals and antiphase or π-spirals. We see that although $E_\pi > E_0$ at low doping, for larger δ it becomes the true semiclassical magnetic ground state of the system.

where

$$F_I(\mathbf{k}) = \xi_2^2(\mathbf{k}) + \xi_0^2(\mathbf{k}) + 2\Delta^2(\mathbf{k}) + \left(\frac{J_K S}{2}\right)^2, \quad (15)$$

and

$$F_{II}(\mathbf{k}) = (\Delta^2(\mathbf{k}) - \xi_2(\mathbf{k})\xi_0(\mathbf{k}))^2 + \left(\frac{J_K S}{2}\right)^2 (\xi_0^2(\mathbf{k}) + \Delta^2(\mathbf{k})). \quad (16)$$

Here

$$\Delta(\mathbf{k}) = t \sin k_y \quad (17)$$

is the CDW gap, with the property $\Delta(\mathbf{k}+\mathbf{q}) = -\Delta(\mathbf{k})$. We see that Eqs. (14) reduce to Eqs. (9) in the limit $\Delta = 0$. For $\Delta \neq 0$, in turn, both $\epsilon_\pi^{(-+)}(\mathbf{k})$ and $\epsilon_\pi^{(--)}(\mathbf{k})$ are always smaller than $\epsilon_0^-(\mathbf{k})$, and thus

$$E_{kin}^\pi = \frac{1}{2}\sum_{\mathbf{k}} \Big\{ \epsilon_\pi^{(-+)}(\mathbf{k})\Theta(\mu - \epsilon_\pi^{(-+)}(\mathbf{k})) + \sum_{\mathbf{k}} \epsilon_\pi^{(--)}(\mathbf{k})\Theta(\mu - \epsilon_\pi^{(--)}(\mathbf{k})) \Big\}, \quad (18)$$

provides us with a rather large gain in kinetic energy. In particular, we found that for $\delta \approx 5\%$, π-spirals already have lower energy than 0-spirals, see Fig. 3. We used units such that $J = 1$, with $t = 3$ and $J_K = 5$, which have the correct hierarchy tipically observed in superconducting cuprates ($J_K > t > J$). As a result, the stabilization of a striped CDW phase coexisting with π-spirals breaks the translational symmetry in the charge sector, gives rise to IC magnetic correlations, and favours 1D trasport *perpendicular* to the spiral pitch.

V. CONCLUSIONS

Using a semiclassical approximation we have revisited the ground state of the SF model. We have shown that π-spirals have lower energy than 0-spirals and give rise to modulated hopping, anisotropic transport, and CDW formation. Thus, although such semiclassical analysis is, strictly speaking, only valid for large S, the possibility of the coexistence of spiral magnetic order and charge modulation is an appealing feature of the new semiclassical ground state here presented, captures the essential physics of the charge and magnetic IC order in $La_{2-x}Sr_xCuO_4$, and has been recently obtained numerically with quantum Monte Carlo.[12] The stability of the semiclassical π-spiral ground state towards fluctuations has still to be demonstrated, but we believe that, as it happens for the case of 0-spirals in the $t-J$ model,[14] the π-spiral phase can also be made robust through the inclusion of next-to-nearest neighbour hopping terms.

The author acknowledges discussions with R. Doretto, C. Morais Smith, A. Moreo, O. Sushkov, and J. Zaanen.

[1] S. Trebst, H. Monien, A. Grzesik, and M. Sigrist, Phys. Rev. B **73**, 165101 (2006).
[2] S. Capponi and F. Assaad, Phys. Rev. B **63**, 155114 (2001).
[3] J. Zaanen and A. Olés, Phys. Rev. B **37**, 4923 (1988).
[4] M. A. Kastner, R. J. Birgeneau, G. Shirane, and Y. Endoh, Rev. Mod. Phys. **70**, 897 (1998).
[5] A. V. Chubukov and K. A. Musaelian, Phys. Rev. B **51**, 12605 (1995).
[6] J. Zaanen and O. Gunnarsson, Phys. Rev. B **40**, 7391 (1989); K. Machida, Physica C **158**, 192 (1989).
[7] B. I. Shraiman and E. D. Siggia, Phys. Rev. B **46**, 8305 (1992).
[8] C. L. Kane, P. A. Lee, T. K. Ng, B. Chakraborty, and N. Read, Phys. Rev. B **41**, 2653 (1990).
[9] K. Yamada *et al.*, Phys. Rev. B **57**, 6165 (1998).
[10] J. M. Tranquada *et al.*, Nature (London) **375**, 561 (1995).
[11] An alternative explanation for the "charge peaks" in $La_{2-x}Sr_xCuO_4$ was recently proposed by the author in Phys. Rev. B **74**, 045109 (2006).
[12] M. Moraghebi, S. Yunoki, and A. Moreo, Phys. Rev. Lett. **88**, 187001 (2002).
[13] M. Hamada and H. Shimahara, Phys. Rev. B **51**, 3027 (1995).
[14] O. P. Sushkov and V. K. Kotov, Phys. Rev. B **70**, 024503 (2004); Phys. Rev. Lett. **94**, 097005 (2005).
[15] V. Juricic, M. B. Silva Neto, and C. Morais Smith, Phys. Rev. Lett. **96**, 077004 (2006).
[16] Y. Liu, J. F. Qu, Y. Q. Zhang, and X. G. Li, Europhys. Lett. **72**, 795 (2005).